Effect of external magnetic field on electron spin dephasing induced by hyperfine interaction in quantum dots

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Abstract

We investigate the influence of an external magnetic field on spin phase relaxation of single electrons in semiconductor quantum dots induced by the hyperfine interaction. The basic decay mechanism is attributed to the dispersion of local effective nuclear fields over the ensemble of quantum dots. The characteristics of electron spin dephasing is analyzed by taking an average over the nuclear spin distribution. We find that the dephasing rate can be estimated as a spin precession frequency caused primarily by the mean value of the local nuclear magnetic field. Furthermore, it is shown that the hyperfine interaction does not fully depolarize electron spin. The loss of initial spin polarization during the dephasing process depends strongly on the external magnetic field, leading to the possibility of effective suppression of this mechanism.

The spin state of an electron confined in a semiconductor quantum dot (QD) is considered one of the most promising candidates for realizing the basic building block (i.e., qubit) of a quantum information system. Since the fundamental concept of this new paradigm relies on quantum mechanical entanglement of qubits, it is quite crucial to control spin relaxation processes that destroy the coherence of spin quantum state. So far, most of the attention has been devoted to the relaxation processes that result in irreversible loss of wave function phase due to spin-phonon interaction caused by spin-orbital coupling in solids or hyperfine interaction (HFI) in crystals with non-zero nuclei spin moments (see Refs. 1 and 2 as well as the references therein). The common feature of these spin-lattice mechanisms is that their relaxation rates are very small in QDs at low temperatures.

On the other hand, the HFI can be considered as a source of a local magnetic field $\overrightarrow{H}_{HF}$ acting on the electron spin that does not disappear at low (or even zero) temperature.[3] This particularity makes the HFI a potentially dominant mehchanism at sufficiently low temperatures. In typical QDs, a sum of the contributions from a great number of nuclei spins forms this field. Thus, the strength and the direction of the $\overrightarrow{H}_{HF}$ are the random variables, which vary from one QD to the next. Obviously, this dispersion can be damaging to quantum computation since electron spin precession occurs with a random phase and frequency. Nevertheless, it appears from a qualitative speculation that the role of $\overrightarrow{H}_{HF}$ dispersion diminishes progressively with an increasing strength of the homogeneous external magnetic field $\overrightarrow{B}$ applied to the array of QDs.

In this paper, we provide a quantitative analysis of electron spin evolution under the presence of an external magnetic field $\overrightarrow{B}$ as well as the local hyperfine field $\overrightarrow{H}_{HF}$. Note, that a theory of electron spin relaxation caused by HFI in a QD was recently presented in Ref. 4. The main interest of Khaetskii *et al.*[4] lies on the electron spin decoherence process inside a single QD when the external magnetic field is zero. It also contains a brief discussion of spin dephasing time. On the other hand, the present study concentrates on the important process of electron spin dephasing induced by HFI in an ensemble of QDs and explicitly considers the effect of external magnetic fields.

The Hamiltonian of electron spin S in a QD containing N nuclear spins I_j ($j = 1, ..., N$) takes the form ($\hbar = 1$)

$$\mathcal{H} = \omega_e S_z + \omega_n \sum_{j=1}^{N} I_{jz} + \sum_{j=1}^{N} A_j \overrightarrow{S} \cdot \overrightarrow{I}_j, \tag{1}$$

where ω_e and ω_n are electron and nuclear spin splitting in a magnetic field directed along the Z axis, A_j is a constant of HFI with the j-th nuclear spin. The Hamiltonian of Eq. (1) is isomorphic to that, which was introduced to describe the bound magnetic polaron in diluted magnetic semiconductors. Most particularities of optical spectroscopy as well as the thermodynamics of bound magnetic polaron were successfully described by a model where differences in constants of spin-spin interaction were ignored.[5,6] By analogy with this model, we describe the dynamics of electron spin by Hamiltonian with a single effective constant A of HFI. This allows one to express the Hamiltonian in terms of the total nuclear spin moment $\vec{F} = \sum_{j=1}^{N} \vec{I}$:

$$\mathcal{H} = \omega_e S_Z + \omega_n F_z + A \overrightarrow{S} \cdot \overrightarrow{F}. \tag{2}$$

Even with such a reduced Hamiltonian, the corresponding equations for the motions of electron and nuclear spins are quite complex,

$$\frac{d}{dt} \left\langle \vec{S} \right\rangle = \overrightarrow{B}_e \times \left\langle \vec{S} \right\rangle + A \left\langle \overrightarrow{F} \times \vec{S} \right\rangle; \tag{3}$$

$$\frac{d}{dt} \left\langle \vec{F} \right\rangle = \overrightarrow{B}_n \times \left\langle \overrightarrow{F} \right\rangle + A \left\langle \vec{S} \times \overrightarrow{F} \right\rangle. \tag{4}$$

where $\overrightarrow{B}_e = \{0, 0, \omega_e\}$ and $\overrightarrow{B}_n = \{0, 0, \omega_n\}$ are in units of energy. Assuming that the flip-flop processes are unimportant for the problem we consider, the Ψ-function of the Hamiltonian given in Eq. (2) can be factorized with respect to electron and nuclear spins. This means that $\left\langle \overrightarrow{F} \times \vec{S} \right\rangle = \left[\left\langle \overrightarrow{F} \right\rangle \times \left\langle \vec{S} \right\rangle \right]$, and Eqs. (3) and (4) present the closed system of equations with respect to $\langle S_\alpha \rangle$ and $\langle F_\alpha \rangle$ ($\alpha = x, y, z$).

Despite the seeming similarity of Eqs. (3) and (4), there is a significant quantitative difference in the effective fields of the nuclei acting on the electron spin $A\overrightarrow{F}$ and of the

electron $\frac{1}{2}A_j$ ($S = 1/2$) acting on the nuclei since a large number $N >> 1$ of nuclear spins are involved in the QD. The latter property with regard to the inequality $\omega_e >> \omega_n$ means a large difference in the typical precession periods for electron and nuclei spins. Thus, for a moment, we can consider the time-dependence of $\left\langle \overrightarrow{F} \right\rangle$ that is given in a parametric representation. The corresponding solution of Eq. (3) with respect to $X(t) \equiv \langle S_X \rangle$, $Y(t) \equiv \langle S_Y \rangle$, $Z(t) \equiv \langle S_Z \rangle$ and initial conditions $X(0) = Y(0) = 0$, $Z(0) = 1/2$ reads

$$X(t) = \frac{AF_x}{2\Omega^2}(AF_z + \omega_e)(1 - \cos\Omega t) + \frac{AF_y}{2\Omega}\sin\Omega t; \tag{5}$$

$$Y(t) = \frac{AF_y}{2\Omega^2}(AF_z + \omega_e)(1 - \cos\Omega t) - \frac{AF_x}{2\Omega}\sin\Omega t; \tag{6}$$

$$Z(t) = \frac{1}{2} - \frac{A^2(F^2 - F_z^2)}{2\Omega^2}(1 - \cos\Omega t). \tag{7}$$

The frequency of electron spin precession

$$\Omega = \sqrt{A^2F^2 + 2AF_z\omega_e + \omega_e^2} \tag{8}$$

has the simple physical meaning of the Zeeman frequency of electron in the total field $\overrightarrow{H}_e = \overrightarrow{B}_e + A\overrightarrow{F}$ composed of external and internal nuclear fields.

Actually, the components of the total nuclear spin moment $F_\alpha(t)$, ($\alpha = x, y, z$) is affected by the external magnetic field $\overrightarrow{B}_n$ and the effective field of an electron $A\left\langle \overrightarrow{S} \right\rangle$, which is oscillating with a high frequency Ω near some mean value $\overline{A\left\langle \overrightarrow{S} \right\rangle}$. This mean value also changes slowly with a typical nuclear frequency $\Omega_n \approx \left|\overrightarrow{B}_n\right| + A/2$. By taking a small interval in time Δt ($<< \Omega_n^{-1}$) to be longer than the period of electron beats (i.e., $\Delta t >> \Omega^{-1}$), one can average over the rapidly oscillating electron contribution in Eq. (4) and arrive at a system of equations with respect to $F_\alpha = F_\alpha(t)$:

$$\frac{d}{dt}F_x = -\omega_n F_y + A\overline{Y(t)}F_z - A\overline{Z(t)}F_y; \tag{9}$$

$$\frac{d}{dt}F_y = \omega_n F_x + A\overline{Z(t)}F_x - A\overline{X(t)}F_z; \tag{10}$$

$$\frac{d}{dt}F_z = A\overline{X(t)}F_y - A\overline{Y(t)}F_x. \tag{11}$$

Here the bars mean the procedure of setting $\sin\Omega t$ and $\cos\Omega t$ to zero when Eqs. (5)-(7) are substituted into Eqs. (9)-(11).

Clearly, Eqs. (9)-(11) are non-linear. Fortunately, we obtain identically zero for the time-derivative $\dot{F}_z = 0$ that provides conservation of the nuclei spin projection F_z on the external magnetic field during the dephasing process described by Eq. (7). Thus, the dispersion of $F = \left|\overrightarrow{F}\right|$ and F_z, caused by the thermal fluctuation in an ensemble of nuclear spins associated with QDs, results in the dephasing of electron spin.

Mathematically, evolution of the spin polarization in an ensemble of QDs can be reduced to the problem of averaging Eq. (7) over the distribution functions for total nuclear spin $[P(F)]$ and for its z-projection $\mu \equiv F_z$ $[P_z(\mu)]$:

$$\langle Z(t)\rangle_T = \int\int Z(t)P_z(\mu)P(F)d\mu dF. \tag{12}$$

The corresponding distribution functions were found in Ref. 5 (see also Ref. 7). In the case of non-saturated nuclear spin polarization, Eq. (12) can be well approximated by the expression

$$\langle Z(t)\rangle_T = C\int_0^{NI} dF \int_{-F}^{F} d\mu F \exp(-\frac{F^2}{\sigma} - \frac{\omega_n \mu}{T})Z(t), \tag{13}$$

where $\sigma = \frac{2}{3}I(I+1)N$ and C is a constant. The averaging in Eq. (13) can be performed numerically for different experimental situations. Some examples of these calculations are presented in Fig. 1 for the case of relatively high temperature $T \gg A\sigma\omega_n/\omega_e$.

Two important conclusions follow immediately from Eqs. (7) and (13) (see also Fig. 1). First, electron spin dephasing does not fully relax its own initial spin polarization $Z_0 = Z(0)$. The minimal rest $Z_\infty = \lim_{t\to\infty}\langle Z(t)\rangle_T$ of Z_0 corresponds to zero magnetic field: $Z_\infty = \frac{1}{3}Z_0$. In a strong enough magnetic field ($B \to \infty$), dephasing will be fully suppressed: $Z_\infty \to Z_0$. Intermediate cases can be traced with high enough accuracy if we substitute high-temperature approximations for the average values of μ and μ^2 in Eq. (13):

$\langle\mu\rangle_T \simeq \frac{1}{3}\langle F^2\rangle \frac{\omega_n}{T} = \frac{\sigma\omega_n}{2T}$ and $\langle\mu^2\rangle_T \simeq \frac{1}{3}\langle F^2\rangle = \frac{\sigma}{2}$. A more detailed approximation is of no interest since it corresponds to saturation of nuclear spin polarization along electron spin polarization that results in insignificant dephasing. The final result reads

$$Z_\infty = \frac{\sigma(\frac{1}{2}A^2 + A\omega_e\frac{\omega_n}{T}) + \omega_e^2}{\sigma(\frac{3}{2}A^2 + A\omega_e\frac{\omega_n}{T}) + \omega_e^2} Z_0. \tag{14}$$

The second conclusion is that dispersion of Zeeman frequency Ω controls the electron dephasing rate. Hence, instead of calculating $\langle Z(t)\rangle_T$ from Eq. (13), we can find the distribution function for Ω; then, the dephasing rate can be estimated as the width of this distribution. In other words, the dephasing rate can be obtained from the width of electron spin resonance lineshape

$$g(\omega) = \int\int \delta(\omega - \Omega) P_z(\mu) P(F) d\mu dF. \tag{15}$$

Using the definitions in Eqs. (13) and (8) as well as the new integrand variables $x = F/\sqrt{\sigma}$, $y = \mu/\sqrt{\sigma}$, Eq. (15) can be rewritten as

$$g(\omega) = C'\omega e^{-\omega^2\tau_0^2} \sinh\left[(2\omega_e\tau_0 + \sqrt{\sigma}\omega_n/T)\omega\tau_0\right]. \tag{16}$$

where $\tau_0 = 1/A\sqrt{\sigma}$. The dephasing rate τ_d^{-1} is expected to be the half width of the $1/e$ decay in the maximal intensity of $g(\omega)$. Equation (16) predicts a weak dependence of τ_d^{-1} on the parameter $2\omega_e\tau_0 + \sqrt{\sigma}\omega_n/T$, which is proportional to the external magnetic field:

$$\tau_d^{-1} = \varphi(2\omega_e\tau_0 + \sqrt{\sigma}\omega_n/T)\tau_0^{-1}, \tag{17}$$

where the function $\varphi(x)$ falls into the region between (0.69,1) (see Fig. 2). Thus, by the order of magnitude, $\tau_d^{-1} \simeq \tau_0^{-1} = A\sqrt{\frac{2}{3}I(I+1)N}$.

At the first glance, it would seem that the efficiency of the phase relaxation increases with the QD volume V_0 as $\sqrt{N} = \sqrt{n_i V_0}$, where n_i is the concentration of isotopes with the nuclear spin I. In actuality, however, we should take into account that the constant of the contact interaction A is proportional to the electron spin density at a nuclear site.[8] As a result, the rate τ_d^{-1} must reveal an inverse dependence on $\sqrt{V_0}$.

Let us estimate the HFI constant A in terms of ENDOR experimental data in Si:P.[9] According to the definition,

$$A = \frac{8\pi}{3} g_e g_n \mu_B \mu_n \left|\Psi\left(\overrightarrow{r}_n\right)\right|^2 \eta. \tag{18}$$

Here g_e and g_n are electron and nuclear g-factors, μ_B and $\mu_n = (m_e/m_p)\,\mu_B$ the Bohr and nuclear magnetons, m_e and m_p the electron and proton masses, $\left|\Psi\left(\overrightarrow{r}_n\right)\right|^2$ is the electron envelope function density at a nuclear lattice site $\overrightarrow{r}_n$, and the parameter η reflects the enhancement of electron density due to the Coulomb singularity at the nuclear core [see, for details, Ref. 3 and Eq. (2.78) therein]. In the case of Si^{29}, this parameter is $\eta = 186$.

To find the parameter A for QD electrons in natural Si, we can use the Feher's experimental data[9] obtained for a shallow donor electron in the presence of Si^{29} separated by $[400]a$ from the donor centrum ($4a = 5.43 \times 10^{-8}$ cm): $A_{400}/2\pi\hbar = 7.72$ MHz. At the same time, the donor electron density $\left|\Psi\left(\overrightarrow{r}_{400}\right)\right|^2$ calculated at this location is $0.4 \times 10^{21}\,\mathrm{cm}^{-3}$. Then, by utilizing the functional form of Eq. (18) that is proportional to the square of the electron density, the HFI constant A at a nuclear site $\overrightarrow{r}_n$ can be expressed as $A = A_{400}\left|\Psi\left(\overrightarrow{r}_n\right)\right|^2 / \left|\Psi\left(\overrightarrow{r}_{400}\right)\right|^2$. If a uniform envelope function is assumed inside the QD, $\Psi\left(\overrightarrow{r}_n\right) = 1/\sqrt{V_0}$, one can find $A/2\pi\hbar = 1.93$ kHz with the QD diameter and thickness of 500 Å and 50 Å, respectively.

Then, in terms of the uniform Ψ-function approximation, we can estimate the number of isotopes Si^{29} in a QD: $N = xV_0/\Omega_0 = 2.29 \times 10^4$, where $x = 0.0467$ is abundance of isotopes Si^{29} and $\Omega_0 = 20$ Å^3 the volume per one Si atom. Thus, one can find $\sigma = \frac{2}{3} I(I+1)N = 1.14 \times 10^4$ and τ_0=0.54×10^{-6} s.

Let us also consider the final loss of electron polarization after dephasing reaches a saturation at $t \gg \tau_0$. According to Eq. (14), the relative loss of initial electron polarization Z_0 is

$$\frac{Z_0 - Z_\infty}{Z_0} = \frac{1}{3/2 + (1+\varepsilon)(\omega_e \tau_0)^2} \tag{19}$$

where $\varepsilon = (\sigma A/T)\,(\omega_n/\omega_e)$. The value of σA which is independent of electron radius localization and abundance of isotopes Si^{29} estimates to be approximately 0.025 K. Thus, with

the exception of extremely low temperatures, we expect the parameter ε to be small.

We can see that Eq. (19) looks similar to that of Hanle effect[3] but with the opposite meaning: increasing magnetic field leads to enhancement (not suppression) of spin polarization. It reflects the competition of random field of nuclei, $H_{HF} = \hbar/g_e\mu_B\tau_0$ (that is on the order of 0.1-1 G in the case of Si QDs), and the external magnetic field B. Accordingly, dephasing is not important if $B \gg H_{HF}$. It is interesting to note that H_{HF} can reach hundred G in QDs composed of III-V semiconductors.[4]

In conclusion, we have considered the influence of an external magnetic field $\vec{B}$ on the electron phase spin relaxation in QDs. The dispersion of nuclear effective local fields $\overrightarrow{H}_{HF}$ over the ensemble of the QDs results in electron spin dephasing. The dephasing rate can be estimated as a spin precession frequency caused by field $\overrightarrow{H}_{HF}$, so it depends weakly on an external magnetic field $\vec{B}$ provided nuclear spin polarization (or magnetization) is not saturated. On the other hand, reduction of electron spin polarization along $\vec{B}$ during the dephasing process does not lead to full depolarization. If the magnetic field is suitably strong, $B \gg H_{HF}$, one can expect an insignificant electron spin depolarization caused by the dephasing process considered.

The result obtained in this study is directly relevant to quantum computing with a large number of qubits (i.e., a large number of QDs containing single electrons). Clearly, random variation in the spin precession frequency and phase across the qubits is deterimental; for example, it can break/negate the initial state preparation in a relatively short time frame of approximately τ_0. Special methods must be applied to compensate this distortion. Our work suggests an effective way to suppress the dispersion of random local fields, making QDs a more attractable candidate for quantum computing.

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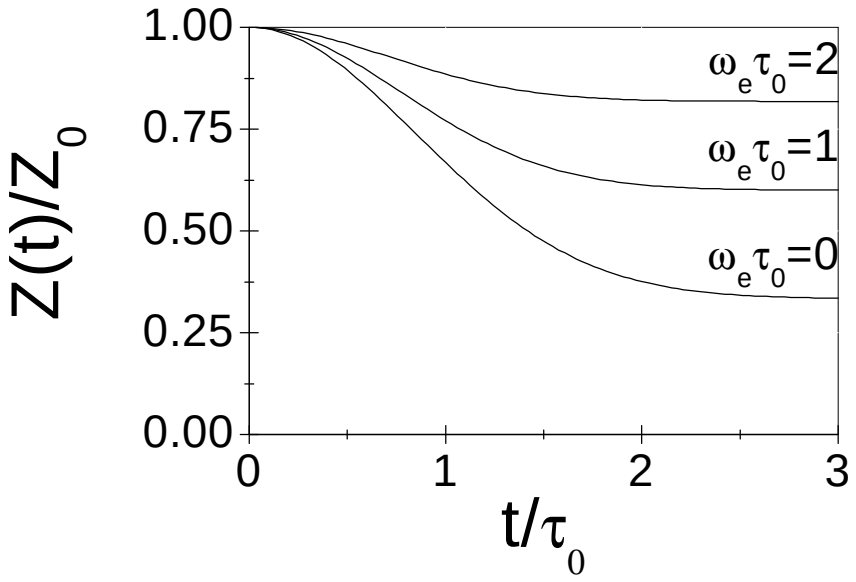
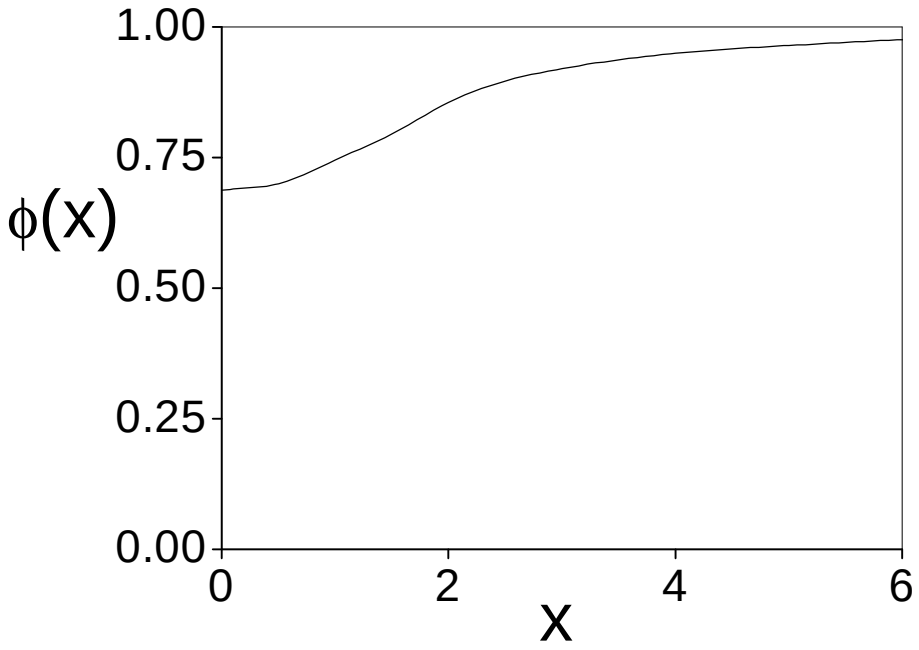
FIGURES

FIG. 1. Spin dephasing of QD electrons calculated for three values of magnetic fields ($\omega_e\tau_0$ =0, 1, and 2). The temperature is assumed to be relatively high: i.e., $T \gg A\sigma\omega_n/\omega_e$ (non-saturated nuclear spin polarization).

FIG. 2. Calculated value of function $\phi(x)$.


1.00
0.75
0.50
0.25
0.00
Z(t)/Z0
0
1
2
3
t/τ0
ωeτ0=2
ωeτ0=1
ωeτ0=0


1.00
0.75
ϕ(x)
0.50
0.25
0.00
0
2
4
6
x